Welcome to STN International! Enter x:x

LOGINID:SSSPTA1623PAZ

PASSWORD:
TERMINAL (ENTER 1, 2, 3, OR ?):2

* * * * * * * * * * Welcome to STN International * * * * * * * * * *

NEWS 1		Web Page for STN Seminar Schedule - N. America
NEWS 2	JUL 28	CA/CAplus patent coverage enhanced
NEWS 3	JUL 28	EPFULL enhanced with additional legal status information from the epoline Register
NEWS 4	JUL 28	IFICDB, IFIPAT, and IFIUDB reloaded with enhancements
NEWS 5	JUL 28	STN Viewer performance improved
NEWS 6	AUG 01	INPADOCDB and INPAFAMDB coverage enhanced
NEWS 7	AUG 13	CA/CAplus enhanced with printed Chemical Abstracts page images from 1967-1998
NEWS 8	AUG 15	CAOLD to be discontinued on December 31, 2008
NEWS 9	AUG 15	CAplus currency for Korean patents enhanced
NEWS 10	AUG 27	CAS definition of basic patents expanded to ensure comprehensive access to substance and sequence information
NEWS 11	SEP 18	Support for STN Express, Versions 6.01 and earlier, to be discontinued
NEWS 12	SEP 25	CA/CAplus current-awareness alert options enhanced to accommodate supplemental CAS indexing of exemplified prophetic substances
NEWS 13	SEP 26	WPIDS, WPINDEX, and WPIX coverage of Chinese and and Korean patents enhanced
NEWS 14	SEP 29	IFICLS enhanced with new super search field
NEWS 15	SEP 29	EMBASE and EMBAL enhanced with new search and display fields
NEWS 16	SEP 30	CAS patent coverage enhanced to include exemplified prophetic substances identified in new Japanese-language patents
NEWS 17	OCT 07	EPFULL enhanced with full implementation of EPC2000
NEWS 18	OCT 07	Multiple databases enhanced for more flexible patent number searching
NEWS 19	OCT 22	Current-awareness alert (SDI) setup and editing enhanced
NEWS 20	OCT 22	WPIDS, WPINDEX, and WPIX enhanced with Canadian PCT Applications
NEWS 21	OCT 24	CHEMLIST enhanced with intermediate list of pre-registered REACH substances

NEWS EXPRESS JUNE 27 08 CURRENT WINDOWS VERSION IS V8.3,
AND CURRENT DISCOVER FILE IS DATED 23 JUNE 2008.

NEWS HOURS	STN Operating Hours Plus Help Desk Availability
NEWS LOGIN	Welcome Banner and News Items
NEWS IPC8	For general information regarding STN implementation of IPC 8

Enter NEWS followed by the item number or name to see news on that specific topic.

  research. Use for software development or design or implementation
  of commercial gateways or other similar uses is prohibited and may
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* * * * * * * * * * * * * * * * STN Columbus * * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 07:05:50 ON 14 NOV 2008

=> ogoff hold
THIS COMMAND NOT AVAILABLE IN THE CURRENT FILE
Some commands only work in certain files. For example, the EXPAND
command can only be used to look at the index in a file which has an
index. Enter "HELP COMMANDS" at an arrow prompt (=>) for a list of
commands which can be used in this file.

=> file reg
COST IN U.S. DOLLARS   SINCE FILE   TOTAL
                                                         ENTRY   SESSION
FULL ESTIMATED COST   0.21   0.21

FILE 'REGISTRY' ENTERED AT 07:06:19 ON 14 NOV 2008
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
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Property values tagged with IC are from the ZIC/VINITI data file
provided by InfoChem.

STRUCTURE FILE UPDATES: 12 NOV 2008 HIGHEST RN 1072189-85-5
DICTIONARY FILE UPDATES: 12 NOV 2008 HIGHEST RN 1072189-85-5

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH July 5, 2008.

  Please note that search-term pricing does apply when
  conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and
predicted properties as well as tags indicating availability of
experimental property data in the original document. For information
on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

=> logoff hold
COST IN U.S. DOLLARS   SINCE FILE   TOTAL
                                                         ENTRY   SESSION
FULL ESTIMATED COST   0.46   0.67

 SESSION WILL BE HELD FOR 120 MINUTES
STN INTERNATIONAL SESSION SUSPENDED AT 07:06:28 ON 14 NOV 2008

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:SSSPTA1623PAZ

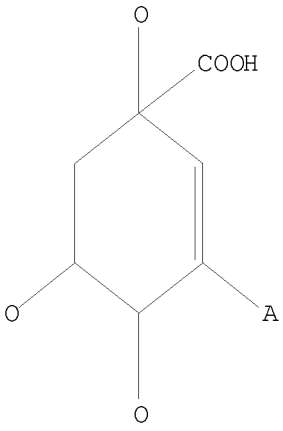
PASSWORD:
 * * * * * * RECONNECTED TO STN INTERNATIONAL * * * * * *
SESSION RESUMED IN FILE 'REGISTRY' AT 07:31:29 ON 14 NOV 2008
FILE 'REGISTRY' ENTERED AT 07:31:29 ON 14 NOV 2008

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.46	0.67

=>
Uploading C:\Documents and Settings\PZucker\My Documents\Examination Auxillary files\10565348\10565348 RCE core.str

L1 STRUCTURE UPLOADED

=> d l1
L1 HAS NO ANSWERS
L1 STR



Structure attributes must be viewed using STN Express query preparation.

=> search l1 sss sam
SAMPLE SEARCH INITIATED 07:32:07 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 252 TO ITERATE

100.0% PROCESSED 252 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 4088 TO 5992
PROJECTED ANSWERS: 0 TO 0

L2 0 SEA SSS SAM L1

=> search l1 sss full
FULL SEARCH INITIATED 07:32:20 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 4961 TO ITERATE

100.0% PROCESSED 4961 ITERATIONS 18 ANSWERS

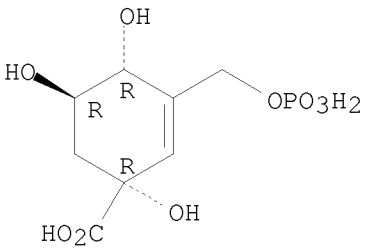
SEARCH TIME: 00.00.01

L3 18 SEA SSS FUL L1

=> d scan

L3 18 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
IN 2-Cyclohexene-1-carboxylic acid, 1,4,5-trihydroxy-3-[(phosphonooxy)methyl]-, (1R,4R,5R)-
MF C8 H13 O9 P

Absolute stereochemistry.

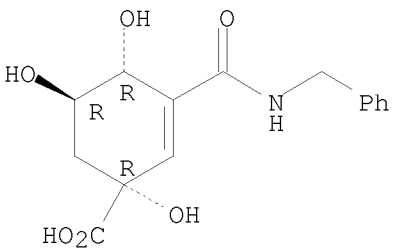


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):18

L3 18 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
IN 2-Cyclohexene-1-carboxylic acid, 1,4,5-trihydroxy-3-[[(phenylmethyl)amino]carbonyl]-, (1R,4R,5R)-
MF C15 H17 N O6

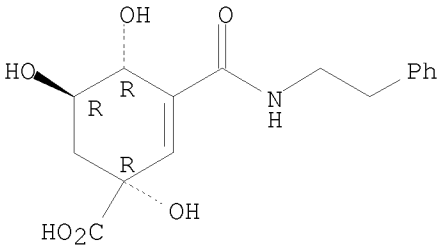
Absolute stereochemistry. Rotation (-).



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 18 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
IN 2-Cyclohexene-1-carboxylic acid, 1,4,5-trihydroxy-3-[[(2-phenylethyl)amino]carbonyl]-, (1R,4R,5R)-
MF C16 H19 N O6

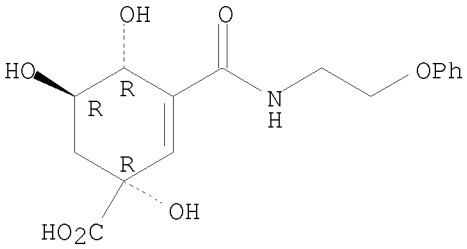
Absolute stereochemistry. Rotation (-).



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 18 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
IN 2-Cyclohexene-1-carboxylic acid, 1,4,5-trihydroxy-3-[[(2-phenoxyethyl)amino]carbonyl]-, (1R,4R,5R)-
MF C16 H19 N O7

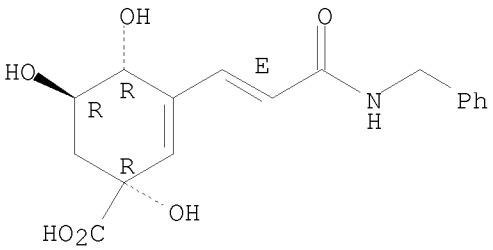
Absolute stereochemistry. Rotation (-).



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 18 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
IN 2-Cyclohexene-1-carboxylic acid, 1,4,5-trihydroxy-3-[(1E)-3-oxo-3-[(phenylmethyl)amino]-1-propen-1-yl]-, (1R,4R,5R)-
MF C17 H19 N O6

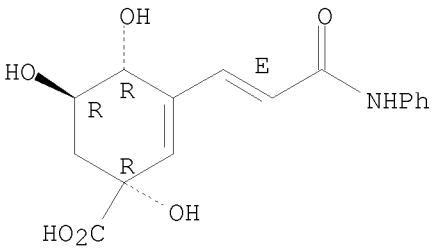
Absolute stereochemistry. Rotation (-).
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 18 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
IN 2-Cyclohexene-1-carboxylic acid, 1,4,5-trihydroxy-3-[(1E)-3-oxo-3-(phenylamino)-1-propen-1-yl]-, (1R,4R,5R)-
MF C16 H17 N O6

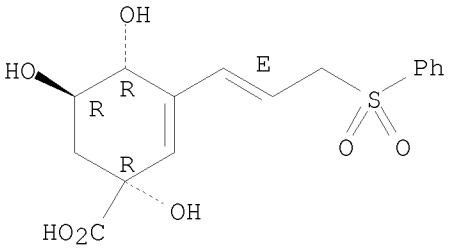
Absolute stereochemistry. Rotation (-).
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 18 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
IN 2-Cyclohexene-1-carboxylic acid, 1,4,5-trihydroxy-3-[(1E)-3-(phenylsulfonyl)-1-propen-1-yl]-, (1R,4R,5R)-
MF C16 H18 O7 S

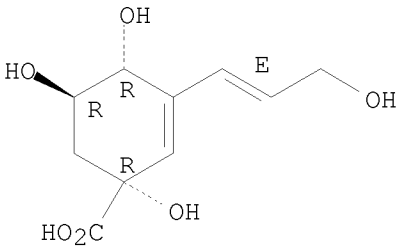
Absolute stereochemistry. Rotation (-).
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 18 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
IN 2-Cyclohexene-1-carboxylic acid, 1,4,5-trihydroxy-3-[(1E)-3-hydroxy-1-propen-1-yl]-, (1R,4R,5R)-
MF C10 H14 O6

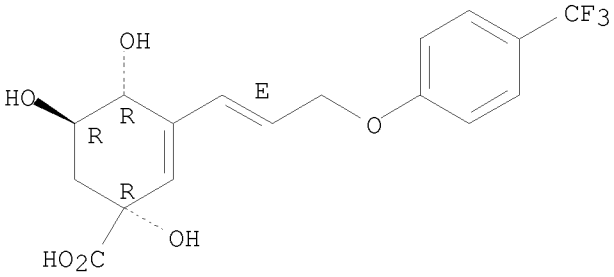
Absolute stereochemistry. Rotation (-).
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3   18 ANSWERS   REGISTRY COPYRIGHT 2008 ACS on STN
IN   2-Cyclohexene-1-carboxylic acid, 1,4,5-trihydroxy-3-[(1E)-3-[4-(trifluoromethyl)phenoxy]-1-propen-1-yl]-, (1R,4R,5R)-
MF   C17 H17 F3 O6

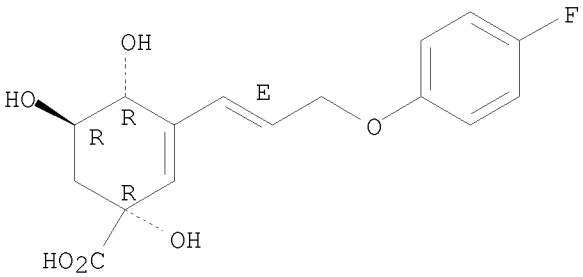
Absolute stereochemistry.
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3   18 ANSWERS   REGISTRY COPYRIGHT 2008 ACS on STN
IN   2-Cyclohexene-1-carboxylic acid, 3-[(1E)-3-(4-fluorophenoxy)-1-propen-1-yl]-1,4,5-trihydroxy-, (1R,4R,5R)-
MF   C16 H17 F O6

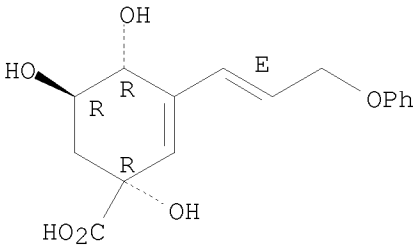
Absolute stereochemistry. Rotation (-).
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 18 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
IN 2-Cyclohexene-1-carboxylic acid, 1,4,5-trihydroxy-3-[(1E)-3-phenoxy-1-propen-1-yl]-, (1R,4R,5R)-
MF C16 H18 O6

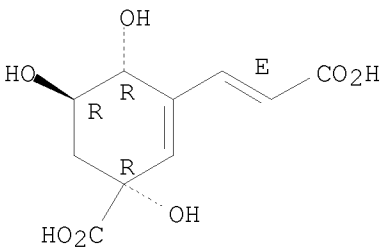
Absolute stereochemistry. Rotation (-).
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 18 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
IN 2-Cyclohexene-1-carboxylic acid, 3-[(1E)-2-carboxyethenyl]-1,4,5-trihydroxy-, (1R,4R,5R)-
MF C10 H12 O7

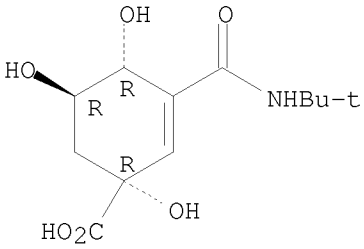
Absolute stereochemistry.
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 18 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
IN 2-Cyclohexene-1-carboxylic acid, 3-[[(1,1-dimethylethyl)amino]carbonyl]-1,4,5-trihydroxy-, (1R,4R,5R)-
MF C12 H19 N O6

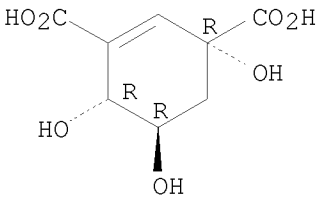
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 18 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
IN 1-Cyclohexene-1,3-dicarboxylic acid, 3,5,6-trihydroxy-, (3R,5R,6R)-
MF C8 H10 O7

Absolute stereochemistry.

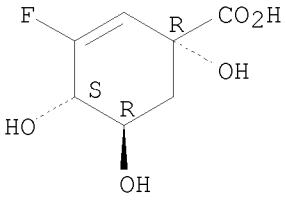


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 18 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
IN 2-Cyclohexene-1-carboxylic acid, 3-fluoro-1,4,5-trihydroxy-, (1R,4S,5R)-

MF C7 H9 F O5

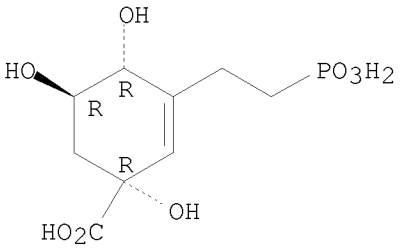
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 18 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
IN 2-Cyclohexene-1-carboxylic acid, 1,4,5-trihydroxy-3-(2-phosphonoethyl)-, (1R,4R,5R)-
MF C9 H15 O8 P

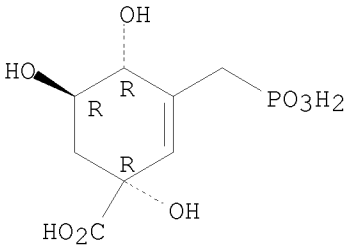
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 18 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
IN 2-Cyclohexene-1-carboxylic acid, 1,4,5-trihydroxy-3-(phosphonomethyl)-, (1R,4R,5R)-
MF C8 H13 O8 P

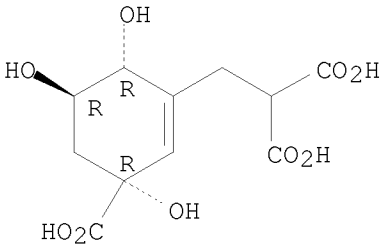
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 18 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
IN Propanedioic acid, 2-[[(3R,5R,6R)-3-carboxy-3,5,6-trihydroxy-1-cyclohexen-1-yl]methyl]-
MF C11 H14 O9

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

ALL ANSWERS HAVE BEEN SCANNED

=> file caplus

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	181.12	181.33

FILE 'CAPLUS' ENTERED AT 07:35:35 ON 14 NOV 2008

FILE COVERS 1907 - 14 Nov 2008 VOL 149 ISS 21
FILE LAST UPDATED: 13 Nov 2008 (20081113/ED)

Caplus now includes complete International Patent Classification (IPC) reclassification data for the second quarter of 2008.

Effective October 17, 2005, revised CAS Information Use Policies apply. They are available for your review at:

```
=> l3
L4           6 L3

=> d l4 1-6 ti fbib abs it
```

L4 ANSWER 1 OF 6 CAPLUS COPYRIGHT 2008 ACS on STN

TI Rational design, synthesis, and evaluation of nanomolar type II dehydroquinase inhibitors

AN 2007:808773 CAPLUS <<LOGINID::20081114>>
DN 147:268289

TI Rational design, synthesis, and evaluation of nanomolar type II dehydroquinase inhibitors

AU Payne, Richard J.; Peyrot, Fabienne; Kerbarh, Olivier; Abell, Andrew D.; Abell, Chris
CS Department of Chemistry, University of Cambridge, Cambridge, CB2 1EW, UK

SO ChemMedChem (2007), 2(7), 1015-1029
CODEN: CHEMGX; ISSN: 1860-7179
PB Wiley-VCH Verlag GmbH & Co. KGaA
DT Journal
LA English
OS CASREACT 147:268289

AB The in silico design, synthesis, and biol. evaluation of ten potent type II dehydroquinase inhibitors are described. These compds. contain an anhydroquinate core, incorporated as a mimic of the enolate reaction intermediate. This substructure is attached by a variety of linking units to a terminal Ph group that binds in an adjacent pocket. Inhibitors were synthesized from (-)-quinic acid using palladium-catalyzed Stille and carboamidation chemical Several inhibitors exhibited nanomolar inhibition consts. against type II dehydroquinases from Streptomyces coelicolor and Mycobacterium tuberculosis. These are among the most potent inhibitors of these enzymes reported to date.

IT Molecular modeling
Mycobacterium tuberculosis
Streptomyces coelicolor
Structure-activity relationship
(anhydroquinate inhibitors of type II dehydroquinase)

IT 9012-66-2, Dehydroquinase
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(anhydroquinate inhibitors of type II dehydroquinase)

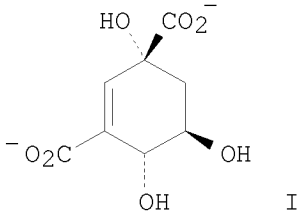
IT 946534-84-5P 946534-85-6P 946534-86-7P
946534-87-8P 946534-88-9P 946534-89-0P
946534-90-3P 946534-91-4P 946534-92-5P
946534-93-6P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(anhydroquinate inhibitors of type II dehydroquinase)

IT 62-53-3, Aniline, reactions 64-04-0, Phenethylamine 100-46-9, Benzylamine, reactions 371-41-5, p-Fluorophenol 402-45-9, p-Trifluoromethylphenol 471-25-0, 2-Propynoic acid 688-73-3, Tributyl tin hydride 813-19-4, Bis(tributyltin) 873-55-2, Sodium phenylsulfinate 1758-46-9, 2-Phenoxyethylamine 13610-02-1 82101-74-4 937184-02-6
RL: RCT (Reactant); RACT (Reactant or reagent)
(anhydroquinate inhibitors of type II dehydroquinase)

IT 7341-97-1P 74141-12-1P 87605-11-6P 119649-71-7P 155197-78-7P
946534-94-7P 946534-95-8P 946534-96-9P 946534-97-0P 946534-98-1P
946534-99-2P 946535-00-8P 946535-01-9P 946535-02-0P 946535-03-1P
946535-04-2P 946535-05-3P 946535-06-4P 946535-07-5P 946535-08-6P

946535-09-7P 946535-10-0P 946535-11-1P 946535-12-2P 946535-13-3P
946535-14-4P 946535-15-5P 946535-16-6P 946535-17-7P 946535-18-8P
946535-19-9P 946535-20-2P 946535-21-3P 946535-22-4P 946535-23-5P
946535-24-6P 946535-25-7P 946535-26-8P 946535-27-9P 946535-28-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(anhydroquinate inhibitors of type II dehydroquinase)
RE.CNT 32 THERE ARE 32 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 2 OF 6 CAPLUS COPYRIGHT 2008 ACS on STN
TI Nanomolar inhibition of type II dehydroquinase based on the enolate reaction mechanism
AN 2007:341043 CAPLUS <<LOGINID::20081114>>
DN 147:671
TI Nanomolar inhibition of type II dehydroquinase based on the enolate reaction mechanism
AU Toscano, Miguel D.; Payne, Richard J.; Chiba, Akira; Kerbarh, Olivier; Abell, Chris
CS Department of Chemistry, University Chemical Laboratory, University of Cambridge, Cambridge, CB2 1EW, UK
SO ChemMedChem (2007), 2(1), 101-112
CODEN: CHEMGX; ISSN: 1860-7179
PB Wiley-VCH Verlag GmbH & Co. KGaA
DT Journal
LA English
OS CASREACT 147:671
GI



I

AB The authors describe the rational design of a novel, highly potent inhibitor of type II dehydroquinase, the dicarboxylate (I). The incorporation of a carboxylate at the 3-position mimics the putative enolate intermediate in the reaction mechanism, and allows a potential electrostatic binding interaction with the arginine on the active site flap. This results in a 1000-fold increase in potency, making the dicarboxylate I the most potent inhibitor of type II dehydroquinase reported to date, with a high ligand efficiency of -0.68 kcal mol-1 per nonhydrogen atom. The systematic dissection of I in compds. 7-12, all of which show a drop in potency, confirm the synergistic importance of the two carboxylates, the C3 and C4 hydroxyl groups, and the anhydroquinate ring structure for the potency of I.
IT Structure-activity relationship
(enzyme-inhibiting; nanomolar inhibition of type II dehydroquinase based on enolate reaction mechanism)
IT Drug design
Molecular association
Molecular modeling
Mycobacterium tuberculosis

Streptomyces coelicolor
(nanomolar inhibition of type II dehydroquinase based on enolate reaction mechanism)
IT Conformation
(protein; nanomolar inhibition of type II dehydroquinase based on enolate reaction mechanism)
IT 937183-95-4P
RL: PAC (Pharmacological activity); PRP (Properties); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(nanomolar inhibition of type II dehydroquinase based on enolate reaction mechanism)
IT 937183-96-5P 937183-97-6P 937183-98-7P 937183-99-8P
937184-00-4P 937184-01-5P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(nanomolar inhibition of type II dehydroquinase based on enolate reaction mechanism)
IT 75-64-9, tert-Butylamine, reactions 109-87-5, Dimethoxymethane
600-22-6, Methyl pyruvate 688-73-3, Tributyltin hydride 813-19-4, Bistributyltin 922-67-8 6089-04-9 7677-24-9, Trimethylsilylcyanide
18448-47-0, Methyl cyclohexene-1-carboxylate 937184-03-7
RL: RCT (Reactant); RACT (Reactant or reagent)
(nanomolar inhibition of type II dehydroquinase based on enolate reaction mechanism)
IT 54396-74-6P 135714-31-7P 189366-37-8P 937184-02-6P 937184-04-8P
937184-05-9P 937184-06-0P 937184-08-2P 937184-09-3P 937184-10-6P
937184-11-7P 937184-12-8P 937184-13-9P 937184-14-0P 937184-15-1P
937184-16-2P 937184-18-4P 937184-19-5P 937184-20-8P 937184-21-9P
937184-22-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(nanomolar inhibition of type II dehydroquinase based on enolate reaction mechanism)
IT 937184-17-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(nanomolar inhibition of type II dehydroquinase based on enolate reaction mechanism)
IT 9012-66-2, Dehydroquinase
RL: BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study)
(type II, inhibitors; nanomolar inhibition of type II dehydroquinase based on enolate reaction mechanism)
RE.CNT 41 THERE ARE 41 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 3 OF 6 CAPLUS COPYRIGHT 2008 ACS on STN
TI Hot off the press
AN 2004:746639 CAPLUS <<LOGINID::20081114>>
DN 142:350581
TI Hot off the press
AU Hill, Robert A.; Sutherland, Andrew
CS Department of Chemistry, Glasgow University, Glasgow, G12 8QQ, UK
SO Natural Product Reports (2004), 21(4), H13-H15
CODEN: NPRRDF; ISSN: 0265-0568
PB Royal Society of Chemistry
DT Journal; General Review
LA English
AB A review covering a selection of 36 recent papers is presented the examines various aspects of current developments in bioorg. chemical and

novel natural products such as bielschowskyin which has a novel diterpenoid framework and shows antimalarial and anticancer activity.

IT Natural products
RL: BIOL (Biological study); OCCU (Occurrence); USES (Uses)
(current developments in bioorg. chemical and novel natural products)

IT 10606-72-1P 128946-78-1P 178948-66-8P
RL: BPN (Biosynthetic preparation); BIOL (Biological study); PREP (Preparation)
(current developments in bioorg. chemical and novel natural products)

IT 50-99-7, D-Glucose, biological studies 1603-79-8 71155-04-9 72909-34-3, Pyrroloquinoline quinone 108605-69-2, Avenanthramide B 486430-83-5 697299-12-0
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(current developments in bioorg. chemical and novel natural products)

IT 51532-30-0, (S)-4-Methyl-3-heptanone 149008-32-2, Phomacta-1(14),3,7-triene 689285-37-8, Mikamicranolide 694440-86-3, Clionastatin A 694440-87-4, Clionastatin B 701203-40-9, Corianlactone 714954-37-7, Psymberin 719296-43-2, Carijenone 719298-06-3, Bisavenanthramide B 720681-08-3, Stolonilactone 720681-62-9, Oxaspirosuberitenone 720685-82-5, Sequosempervirin A 742088-25-1, Gymnorrhizol 790710-32-6, Spirodepressolide
RL: BSU (Biological study, unclassified); NPO (Natural product occurrence); BIOL (Biological study); OCCU (Occurrence)
(current developments in bioorg. chemical and novel natural products)

IT 697298-90-1, Bielschowskysin
RL: BSU (Biological study, unclassified); NPO (Natural product occurrence); PAC (Pharmacological activity); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); OCCU (Occurrence); USES (Uses)
(current developments in bioorg. chemical and novel natural products)

IT 677025-48-8, Menisporopsin A 681456-07-5 682334-57-2, Brasilienosophyllic acid A 725254-09-1, Abyssomicin C
RL: BSU (Biological study, unclassified); NPO (Natural product occurrence); PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); OCCU (Occurrence); USES (Uses)
(current developments in bioorg. chemical and novel natural products)

IT 339541-50-3, Prerapamycin 360555-98-2, Spongidepsin
RL: BSU (Biological study, unclassified); NPO (Natural product occurrence); PRP (Properties); BIOL (Biological study); OCCU (Occurrence)
(current developments in bioorg. chemical and novel natural products)

L4 ANSWER 4 OF 6 CAPLUS COPYRIGHT 2008 ACS on STN

TI (1R,4S,5R)-3-Fluoro-1,4,5-trihydroxy-2-cyclohexene-1-carboxylic acid: the fluoro analogue of the enolate intermediate in the reaction catalyzed by type II dehydroquinases

AN 2004:422880 CAPLUS <<LOGINID::20081114>>

DN 141:140692

TI (1R,4S,5R)-3-Fluoro-1,4,5-trihydroxy-2-cyclohexene-1-carboxylic acid: the fluoro analogue of the enolate intermediate in the reaction catalyzed by type II dehydroquinases

AU Frederickson, Martyn; Roszak, Aleksander W.; Coggins, John R.; Lapthorn, Adrian J.; Abell, Chris

CS University Chemical Laboratory, Cambridge, CB2 1EW, UK

SO Organic & Biomolecular Chemistry (2004), 2(11), 1592-1596
CODEN: OBCRAK; ISSN: 1477-0520

PB Royal Society of Chemistry

DT Journal

LA English

OS CASREACT 141:140692

AB The fluoro analog of the enolate intermediate in the reaction catalyzed by type II dehydroquinases has been prepared from naturally occurring (-)-quinic acid over seven steps and has been shown to be the most potent

inhibitor reported to date of the type II enzyme from Mycobacterium tuberculosis.

IT Cyclitols
RL: BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(fluoro; preparation of (1R,4S,5R)-3-fluoro-1,4,5-trihydroxy-2-cyclohexene-1-carboxylic acid analogs and their inhibition of bacterial dehydroquinases)

IT Mycobacterium tuberculosis
(preparation of (1R,4S,5R)-3-fluoro-1,4,5-trihydroxy-2-cyclohexene-1-carboxylic acid analogs and their inhibition of bacterial dehydroquinases)

IT 9012-66-2
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(preparation of (1R,4S,5R)-3-fluoro-1,4,5-trihydroxy-2-cyclohexene-1-carboxylic acid analogs and their inhibition of bacterial dehydroquinases)

IT 13019-10-8P 486430-83-5P 486430-84-6P
RL: BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation of (1R,4S,5R)-3-fluoro-1,4,5-trihydroxy-2-cyclohexene-1-carboxylic acid analogs and their inhibition of bacterial dehydroquinases)

IT 177284-79-6P 725738-25-0P
RL: PNU (Preparation, unclassified); PREP (Preparation)
(preparation of (1R,4S,5R)-3-fluoro-1,4,5-trihydroxy-2-cyclohexene-1-carboxylic acid analogs and their inhibition of bacterial dehydroquinases)

IT 77-95-2, (-)-Quinic acid 177284-85-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of (1R,4S,5R)-3-fluoro-1,4,5-trihydroxy-2-cyclohexene-1-carboxylic acid analogs and their inhibition of bacterial dehydroquinases)

IT 176798-26-8P 183474-88-6P 183475-04-9P 486430-85-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of (1R,4S,5R)-3-fluoro-1,4,5-trihydroxy-2-cyclohexene-1-carboxylic acid analogs and their inhibition of bacterial dehydroquinases)

IT 177284-86-5P 177284-87-6P 486430-86-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of (1R,4S,5R)-3-fluoro-1,4,5-trihydroxy-2-cyclohexene-1-carboxylic acid analogs and their inhibition of bacterial dehydroquinases)

RE.CNT 38 THERE ARE 38 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 5 OF 6 CAPLUS COPYRIGHT 2008 ACS on STN
TI Vinyl fluoride as an isoelectronic replacement for an enolate anion: Inhibition of type II dehydroquinases
AN 2002:647422 CAPLUS <<LOGINID::20081114>>
DN 138:102740
TI Vinyl fluoride as an isoelectronic replacement for an enolate anion: Inhibition of type II dehydroquinases
AU Frederickson, Martyn; Coggins, John R.; Abell, Chris
CS University Chemical Laboratory, Cambridge, CB2 1EW, UK
SO Chemical Communications (Cambridge, United Kingdom) (2002), (17), 1886-1887
CODEN: CHCOFS; ISSN: 1359-7345
PB Royal Society of Chemistry

DT Journal
LA English
OS CASREACT 138:102740
AB A vinyl fluoride analog of the intermediate in the reaction catalyzed by type II dehydroquinase enzymes has been synthesized over seven steps from (-)-quinic acid and shown to be a potent enzyme inhibitor.
IT Enzyme kinetics
(of inhibition; vinyl fluoride analog as isoelectronic replacement for an enolate anion and inhibitor of type II dehydroquinases)
IT Crystal structure
(vinyl fluoride analog as isoelectronic replacement for an enolate anion and inhibitor of type II dehydroquinases)
IT 486430-86-8P
RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(crystal structure properties; vinyl fluoride analog as isoelectronic replacement for an enolate anion and inhibitor of type II dehydroquinases)
IT 486430-83-5P
RL: BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(vinyl fluoride analog as isoelectronic replacement for an enolate anion and inhibitor of type II dehydroquinases)
IT 77-95-2, (-)-Quinic acid 109-87-5 149-73-5 176798-33-7 227002-11-1
RL: RCT (Reactant); RACT (Reactant or reagent)
(vinyl fluoride analog as isoelectronic replacement for an enolate anion and inhibitor of type II dehydroquinases)
IT 176798-26-8P 183474-88-6P 183475-04-9P 486430-85-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(vinyl fluoride analog as isoelectronic replacement for an enolate anion and inhibitor of type II dehydroquinases)
IT 486430-84-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(vinyl fluoride analog as isoelectronic replacement for an enolate anion and inhibitor of type II dehydroquinases)
IT 9012-66-2, E.C. 4.2.1.10
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(vinyl fluoride as an isoelectronic replacement for an enolate anion: inhibition of type II dehydroquinases)
RE.CNT 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 6 OF 6 CAPLUS COPYRIGHT 2008 ACS on STN
TI Cyclohexenyl and Cyclohexylidene Inhibitors of 3-Dehydroquinate Synthase: Active Site Interactions Relevant to Enzyme Mechanism and Inhibitor Design
AN 1997:528717 CAPLUS <<LOGINID::20081114>>
DN 127:216861
OREF 127:42125a,42128a
TI Cyclohexenyl and Cyclohexylidene Inhibitors of 3-Dehydroquinate Synthase: Active Site Interactions Relevant to Enzyme Mechanism and Inhibitor Design
AU Montchamp, Jean-Luc; Frost, J. W.
CS Contribution from the Department of Chemistry, Michigan State University, East Lansing, MI, 48824, USA
SO Journal of the American Chemical Society (1997), 119(33), 7645-7653
CODEN: JACSAT; ISSN: 0002-7863
PB American Chemical Society
DT Journal
LA English
AB Cyclohexenyl and cyclohexylidene inhibitors possessing strategically placed olefinic residues, in general, bind to 3-dehydroquinate (DHQ)

synthase more tightly than similarly substituted cyclohexyl inhibitors. All of the newly synthesized inhibitors were prepared from a common DHQ derivative Cyclohexenyl phosphate 1 is the most potent inhibitor of DHQ synthase thus far identified with an inhibition constant (Ki = 1.2+10-10 M), indicating active site binding 1000-fold tighter relative to the corresponding cyclohexyl phosphate 5. Cyclohexenyl tricarboxylate 2 binds 700-fold more tightly than similarly substituted cyclohexyl tricarboxylate 6 and is the first example of a nanomolar-level inhibitor (Ki = 8.6+10-9 M) possessing neither a phosphate monoester or a phosphonic acid. Cyclohexenyl homophosphonate 4 (Ki = 3.0+10-8 M) and cyclohexylidene homophosphonate 10 (Ki = 3.2+10-9 M) bind 57- and 530-fold, resp., more tightly than the corresponding cyclohexyl homophosphonate 8. Cyclohexylidene homophosphonate 10 is the first example of a nanomolar-level, homophosphonic acid inhibitor of DHQ synthase. Cyclohexylidene phosphonate 9 (Ki = 2.9+10-10 M) is a 2.9-fold more potent inhibitor relative to cyclohexyl phosphonate 7 which was previously the most potent, slowly-reversible inhibitor of DHQ synthase. Cyclohexenyl phosphonate 3 (Ki = 1.2+10-9 M) is the only olefin-containing, carbocyclic inhibitor where improved binding over the corresponding cyclohexyl analog was not observed The impact of olefinic residues in inhibitors on active site binding may indicate that DHQ synthase plays an active catalytic role during E1cb elimination of inorg. phosphate from enzyme-bound substrate.

IT Enzyme kinetics
(design and preparation of cyclohexenyl and cyclohexylidene inhibitors of 3-dehydroquinate synthase)

IT Structure-activity relationship
(enzyme-inhibiting, 3-dehydroquinate synthase; design and preparation of cyclohexenyl and cyclohexylidene inhibitors of 3-dehydroquinate synthase)

IT 119480-86-3 119480-87-4 123075-71-8
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(design and preparation of cyclohexenyl and cyclohexylidene inhibitors of 3-dehydroquinate synthase)

IT 194998-86-2P 194998-87-3P 194998-88-4P
194998-89-5P 194998-90-8P 194998-91-9P 194998-92-0P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(design and preparation of cyclohexenyl and cyclohexylidene inhibitors of 3-dehydroquinate synthase)

IT 37211-77-1, 3-Dehydroquinate synthase
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(design and preparation of cyclohexenyl and cyclohexylidene inhibitors of 3-dehydroquinate synthase)

IT 77-95-2
RL: RCT (Reactant); RACT (Reactant or reagent)
(design and preparation of cyclohexenyl and cyclohexylidene inhibitors of 3-dehydroquinate synthase)

IT 176798-26-8P 183474-88-6P 194998-93-1P 194998-94-2P 194998-95-3P
194998-96-4P 194998-97-5P 194998-98-6P 194998-99-7P 194999-00-3P
194999-01-4P 194999-02-5P 194999-03-6P 194999-04-7P 194999-05-8P
194999-06-9P 194999-07-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(design and preparation of cyclohexenyl and cyclohexylidene inhibitors of 3-dehydroquinate synthase)

RE.CNT 46 THERE ARE 46 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> 486430-83-5
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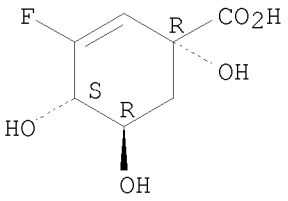
L6   3 L5

=> display hitstr l6 1-3

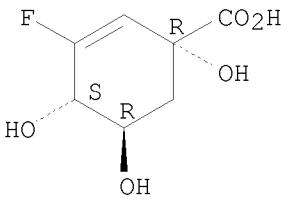
L6   ANSWER 1 OF 3 CAPLUS COPYRIGHT 2008 ACS on STN
IT   486430-83-5
     RL: BSU (Biological study, unclassified); BIOL (Biological study)
        (current developments in bioorg. chemical and novel natural products)
RN   486430-83-5 CAPLUS
CN   2-Cyclohexene-1-carboxylic acid, 3-fluoro-1,4,5-trihydroxy-, (1R,4S,5R)-
     (CA INDEX NAME)

Absolute stereochemistry.



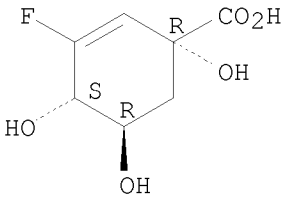
L6   ANSWER 2 OF 3 CAPLUS COPYRIGHT 2008 ACS on STN
IT   486430-83-5P
     RL: BSU (Biological study, unclassified); SPN (Synthetic preparation);
     BIOL (Biological study); PREP (Preparation)
        (preparation of (1R,4S,5R)-3-fluoro-1,4,5-trihydroxy-2-cyclohexene-1-
        carboxylic acid analogs and their inhibition of bacterial
        dehydroquinases)
RN   486430-83-5 CAPLUS
CN   2-Cyclohexene-1-carboxylic acid, 3-fluoro-1,4,5-trihydroxy-, (1R,4S,5R)-
     (CA INDEX NAME)

Absolute stereochemistry.



L6 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2008 ACS on STN
IT 486430-83-5P
    RL: BSU (Biological study, unclassified); SPN (Synthetic preparation);
    BIOL (Biological study); PREP (Preparation)
       (vinyl fluoride analog as isoelectronic replacement for an enolate
       anion and inhibitor of type II dehydroquinases)
RN 486430-83-5 CAPLUS
CN 2-Cyclohexene-1-carboxylic acid, 3-fluoro-1,4,5-trihydroxy-, (1R,4S,5R)-
    (CA INDEX NAME)

Absolute stereochemistry.



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experimental property data in the original document. For information
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http://www.cas.org/support/stngen/stndoc/properties.html

=> e 2-Cyclohexene-1-carboxylic acid,
1,4,5-trihydroxy-3-((1E)-3-hydroxy-1-propen-1-yl)-, (1R,4R,5R)-/cn

```
E1            1     2-CYCLOHEXENE-1-CARBOXYLIC ACID, 1,4,5-TRIHYDROXY-3-((1E)-3-
                    (4-(TRIFLUOROMETHYL)PHENOXY)-1-PROPEN-1-YL)-, (1R,4R,5R)-/CN
E2            1     2-CYCLOHEXENE-1-CARBOXYLIC ACID, 1,4,5-TRIHYDROXY-3-((1E)-3-
                    (PHENYLSULFONYL)-1-PROPEN-1-YL)-, (1R,4R,5R)-/CN
E3            1 --> 2-CYCLOHEXENE-1-CARBOXYLIC ACID, 1,4,5-TRIHYDROXY-3-((1E)-3-
                    HYDROXY-1-PROPEN-1-YL)-, (1R,4R,5R)-/CN
E4            1     2-CYCLOHEXENE-1-CARBOXYLIC ACID, 1,4,5-TRIHYDROXY-3-((1E)-3-
                    OXO-3-((PHENYLMETHYL)AMINO)-1-PROPEN-1-YL)-, (1R,4R,5R)-/CN
E5            1     2-CYCLOHEXENE-1-CARBOXYLIC ACID, 1,4,5-TRIHYDROXY-3-((1E)-3-
                    OXO-3-(PHENYLAMINO)-1-PROPEN-1-YL)-, (1R,4R,5R)-/CN
E6            1     2-CYCLOHEXENE-1-CARBOXYLIC ACID, 1,4,5-TRIHYDROXY-3-((1E)-3-
                    PHENOXY-1-PROPEN-1-YL)-, (1R,4R,5R)-/CN
E7            1     2-CYCLOHEXENE-1-CARBOXYLIC ACID, 1,4,5-TRIHYDROXY-3-((PHOSPH
                    ONOOXY)METHYL)-, (1R,4R,5R)-/CN
E8            1     2-CYCLOHEXENE-1-CARBOXYLIC ACID, 1,4,5-TRIHYDROXY-3-((PHOSPH
                    ONOOXY)METHYL)-, (1R-(1A,4A,5B))-/CN
E9            1     2-CYCLOHEXENE-1-CARBOXYLIC ACID, 1,4,5-TRIHYDROXY-3-(1-(PHEN
                    YLMETHYL)-1H-1,2,3-TRIAZOL-4-YL)-, (1R,4R,5R)-/CN
E10           1     2-CYCLOHEXENE-1-CARBOXYLIC ACID, 1,4,5-TRIHYDROXY-3-(1H-1,2,
                    3-TRIAZOL-5-YL)-, (1R,4R,5R)-/CN
E11           1     2-CYCLOHEXENE-1-CARBOXYLIC ACID, 1,4,5-TRIHYDROXY-3-(1H-INDO
                    L-6-YL)-, (1R,4R,5R)-/CN
E12           1     2-CYCLOHEXENE-1-CARBOXYLIC ACID, 1,4,5-TRIHYDROXY-3-(2-NAPHT
                    HALENYL)-, (1R,4R,5R)-/CN

=> e3
L7            1 "2-CYCLOHEXENE-1-CARBOXYLIC ACID, 1,4,5-TRIHYDROXY-3-((1E)-3-HYD
                ROXY-1-PROPEN-1-YL)-, (1R,4R,5R)-"/CN

=> d l7

L7   ANSWER 1 OF 1  REGISTRY  COPYRIGHT 2008 ACS on STN
RN   946534-87-8  REGISTRY
ED   Entered STN:  10 Sep 2007
CN   2-Cyclohexene-1-carboxylic acid,
     1,4,5-trihydroxy-3-[(1E)-3-hydroxy-1-propen-1-yl]-, (1R,4R,5R)-  (CA
     INDEX NAME)
FS   STEREOSEARCH
MF   C10 H14 O6
SR   CA
LC   STN Files:   CA, CAPLUS, CASREACT

Absolute stereochemistry.  Rotation (-).
Double bond geometry as shown.
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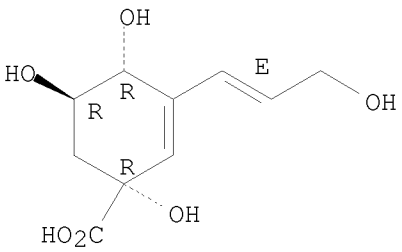


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1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

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=> l7
L8 1 L7

=> d l8 ti fbib abs it

L8 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2008 ACS on STN
TI Rational design, synthesis, and evaluation of nanomolar type II dehydroquinase inhibitors
AN 2007:808773 CAPLUS <<LOGINID::20081114>>
DN 147:268289
TI Rational design, synthesis, and evaluation of nanomolar type II dehydroquinase inhibitors
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SO ChemMedChem (2007), 2(7), 1015-1029
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DT Journal
LA English
OS CASREACT 147:268289
AB The in silico design, synthesis, and biol. evaluation of ten potent type II dehydroquinase inhibitors are described. These compds. contain an anhydroquinate core, incorporated as a mimic of the enolate reaction intermediate. This substructure is attached by a variety of linking units to a terminal Ph group that binds in an adjacent pocket. Inhibitors were synthesized from (-)-quinic acid using palladium-catalyzed Stille and carboamidation chemical Several inhibitors exhibited nanomolar inhibition consts. against type II dehydroquinases from Streptomyces coelicolor and Mycobacterium tuberculosis. These are among the most potent inhibitors of these enzymes reported to date.
IT Molecular modeling
Mycobacterium tuberculosis
Streptomyces coelicolor
Structure-activity relationship
(anhydroquinate inhibitors of type II dehydroquinase)
IT 9012-66-2, Dehydroquinase
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(anhydroquinate inhibitors of type II dehydroquinase)
IT 946534-84-5P 946534-85-6P 946534-86-7P 946534-87-8P
946534-88-9P 946534-89-0P 946534-90-3P 946534-91-4P 946534-92-5P
946534-93-6P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(anhydroquinate inhibitors of type II dehydroquinase)
IT 62-53-3, Aniline, reactions 64-04-0, Phenethylamine 100-46-9, Benzylamine, reactions 371-41-5, p-Fluorophenol 402-45-9, p-Trifluoromethylphenol 471-25-0, 2-Propynoic acid 688-73-3, Tributyl tin hydride 813-19-4, Bis(tributyltin) 873-55-2, Sodium phenylsulfinate 1758-46-9, 2-Phenoxyethylamine 13610-02-1 82101-74-4
937184-02-6
RL: RCT (Reactant); RACT (Reactant or reagent)
(anhydroquinate inhibitors of type II dehydroquinase)
IT 7341-97-1P 74141-12-1P 87605-11-6P 119649-71-7P 155197-78-7P
946534-94-7P 946534-95-8P 946534-96-9P 946534-97-0P 946534-98-1P
946534-99-2P 946535-00-8P 946535-01-9P 946535-02-0P 946535-03-1P
946535-04-2P 946535-05-3P 946535-06-4P 946535-07-5P 946535-08-6P
946535-09-7P 946535-10-0P 946535-11-1P 946535-12-2P 946535-13-3P
946535-14-4P 946535-15-5P 946535-16-6P 946535-17-7P 946535-18-8P
946535-19-9P 946535-20-2P 946535-21-3P 946535-22-4P 946535-23-5P
946535-24-6P 946535-25-7P 946535-26-8P 946535-27-9P 946535-28-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(anhydroquinate inhibitors of type II dehydroquinase)
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